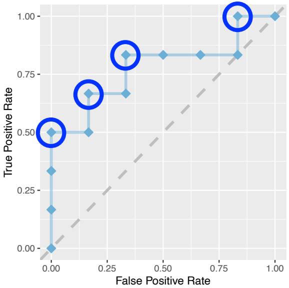
Introduction to Machine Learning

Evaluation: Measures for Binary Classification: ROC Visualization

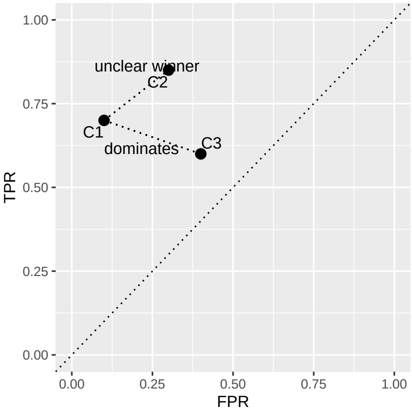


Learning goals

- Understand ROC curve
- Be able to compute a ROC curve manually
- Understand that ROC curve is invariant to class priors at test-time
- Discuss threshold selection
- Understand AUC

LABELS: ROC SPACE

- For comparing classifiers, we characterize them by their TPR and FPR values and plot them in a coordinate system.
- We could also use two different ROC metrics which define a trade-off, for instance, TPR and PPV.



		True Class y	
		$+$	$-$
Pred.	$+$	TP	FP
$\hat{y}$	$-$	FN	TN

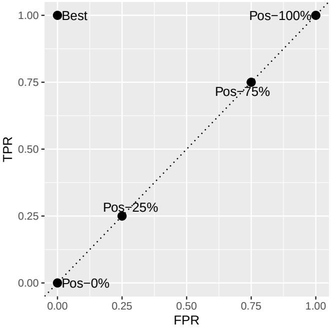
$$\text{TPR} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

$$\text{FPR} = \frac{\text{FP}}{\text{FP} + \text{TN}}$$

LABELS: ROC SPACE

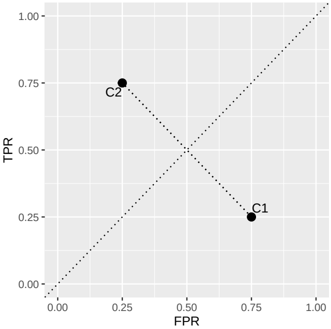
- The best classifier lies on the top-left corner, where FPR equals 0 and TPR is maximal.
- The diagonal is worst as it corresponds to a classifier producing random labels (with different proportions).

- If each positive x will be randomly classified with 25% as "pos", $\text{TPR} = 0.25$.
- If we assign each negative x randomly to "pos", $\text{FPR} = 0.25$.



LABELS: ROC SPACE

- In practice, we should never obtain a classifier below the diagonal.
- Inverting the predicted labels ($0 \mapsto 1$ and $1 \mapsto 0$) will result in a reflection at the diagonal.
  $\Rightarrow \text{TPR}_{\text{new}} = 1 - \text{TPR}$ and $\text{FPR}_{\text{new}} = 1 - \text{FPR}$.



LABEL DISTRIBUTION IN TPR AND FPR

TPR and FPR (ROC curves) are insensitive to the class distribution in the sense that they are not affected by changes in the ratio n_+/n_- (at prediction).

Example 1:
Proportion $n_+/n_- = 1$

	Actual Positive	Actual Negative
Pred. Positive	40	25
Pred. Negative	10	25

$\text{MCE} = 35/100 = 0.35$
$\text{TPR} = 0.8$
$\text{FPR} = 0.5$

Example 2:
Proportion $n_+/n_- = 2$

	Actual Positive	Actual Negative
Pred. Positive	80	25
Pred. Negative	20	25

$\text{MCE} = 45/150 = 0.3$
$\text{TPR} = 0.8$
$\text{FPR} = 0.5$

Note: If class proportions differ during training, the above is not true. Estimated posterior probabilities can change!

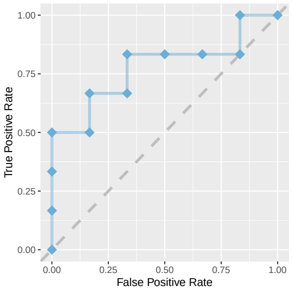
FROM PROBABILITIES TO LABELS: ROC CURVE

Remember: Both probabilistic and scoring classifiers can output classes by thresholding:

$$h(\mathbf{x}) = [\pi(\mathbf{x}) \geq c] \quad \text{or} \quad h(\mathbf{x}) = [f(\mathbf{x}) \geq c_f].$$

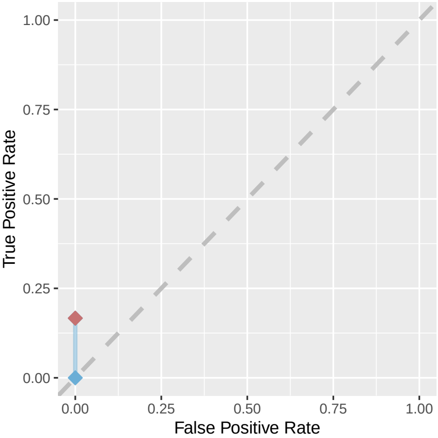
To draw a ROC curve:

1. Rank test observations on decreasing score.
2. Start with $c = 1$, so we start in $(0, 0)$; we predict everything as negative.
3. Iterate through all possible thresholds c and proceed for each observation x as follows:
   - If x is positive, move TPR $1/n_+$ up, as we have one TP more.
   - If x is negative, move FPR $1/n_-$ right, as we have one FP more.

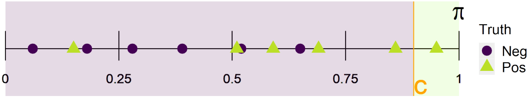


DRAWING ROC CURVES

#	Truth	Score
1	Pos	0.95
2	Pos	0.86
3	Pos	0.69
4	Neg	0.65
5	Pos	0.59
6	Neg	0.52
7	Pos	0.51
8	Neg	0.39
9	Neg	0.28
10	Neg	0.18
11	Pos	0.15
12	Neg	0.06



$c = 0.9$
$\rightarrow$ TPR = 0.167
$\rightarrow$ FPR = 0



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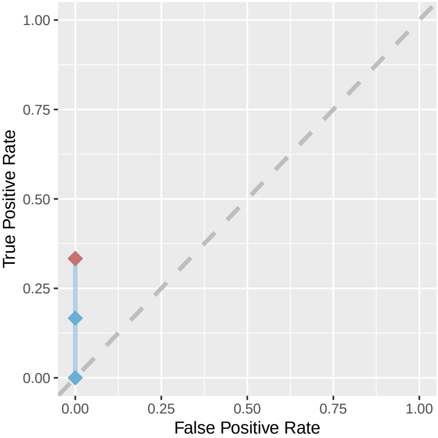
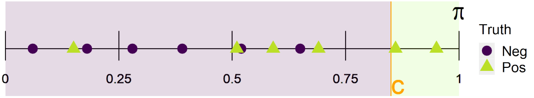


$c = 0.85$

$\rightarrow$ TPR = 0.333

$\rightarrow$ FPR = 0



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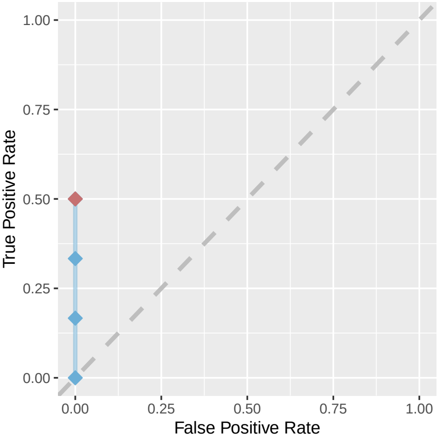
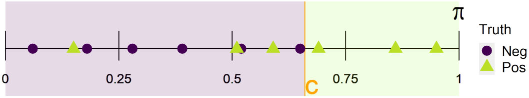


$c = 0.66$
$\rightarrow$ TPR = 0.5
$\rightarrow$ FPR = 0



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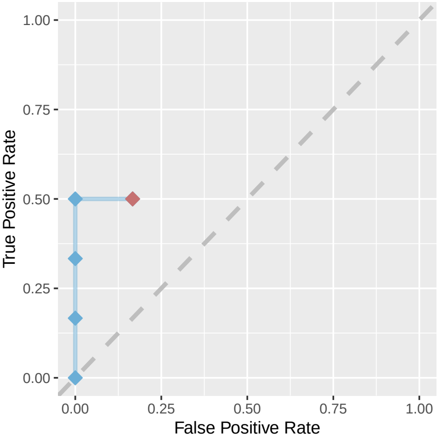
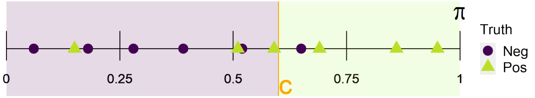


$c = 0.6$

$\rightarrow$ TPR = 0.5

$\rightarrow$ FPR = 0.167



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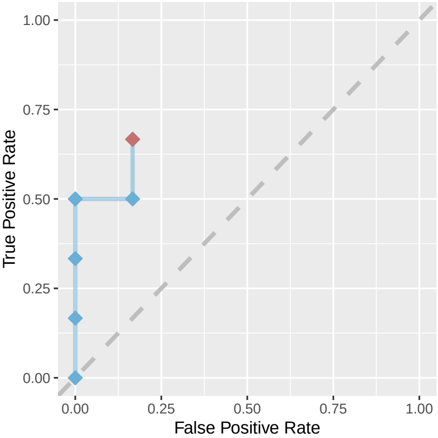
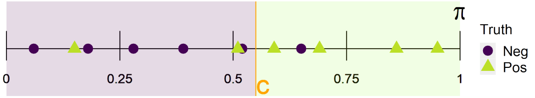


$c = 0.55$

$\rightarrow$ TPR = 0.667

$\rightarrow$ FPR = 0.167



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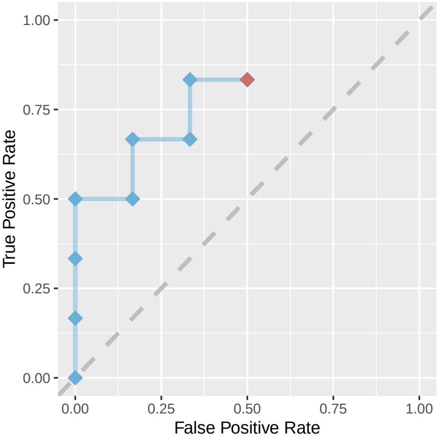
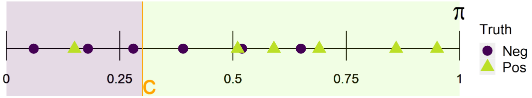


$c = 0.3$

$\rightarrow$ TPR = 0.833

$\rightarrow$ FPR = 0.5



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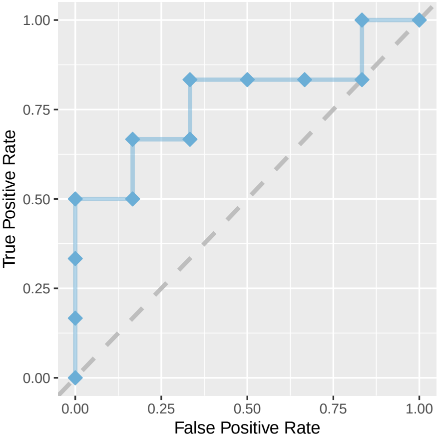
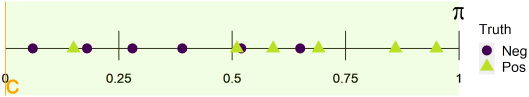


$c = 0$

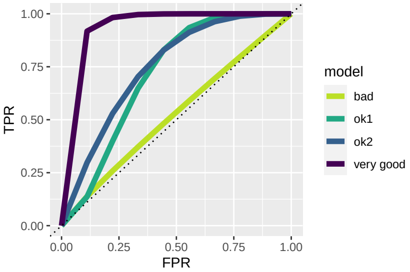
$\rightarrow$ TPR = 1

$\rightarrow$ FPR = 1



ROC CURVE PROPERTIES

- The closer the curve to the top-left corner, the better.
- If ROC curves cross, a different model might be better in different parts of the ROC space.

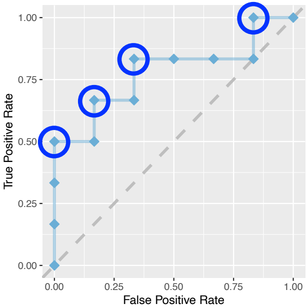


- Small thresholds will very liberally predict the positive class, and result in a potentially higher FPR, but also higher TPR.
- High thresholds will very conservatively predict the positive class, and result in a lower FPR and TPR.
- As we have not defined the trade-off between false positive and false negative costs, we cannot easily select the "best" threshold.
  $\rightarrow$ Visual inspection of all possible results seems useful.

CHOOSING THRESHOLD / OPERATING POINT

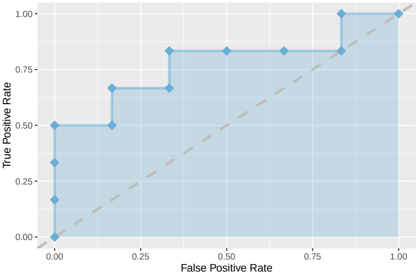
Often done visually and post-hoc, as class imbalances or costs are unknown a-priori.

- Identify non-dominated points
- Assess TPR / FPR
- Decide which combo is best for task
- Pick associated threshold



AUC: AREA UNDER ROC CURVE

- AUC $\in [0, 1]$ is a single metric to evaluate scoring classifiers – independent of the chosen threshold.
  - AUC = 1: perfect classifier
  - AUC = 0.5: random, non-discriminant classifier
  - AUC = 0: perfect, with inverted labels



AUC AS A RANK-BASED METRIC

- We can also interpret the AUC as the probability of our classifier ranking a random positive observation higher than a random negative one.
- A perfect classifier will rank all positive above all negative observations, achieving AUC = 1.